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DESIGN OF A TENSOR PRODUCT POPULATION OF PDE PROBLEMS

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ABSTRACT

We present the design of a population of problems for the scientific evaluation of software for solving partial differential equations (PDEs). The design provides both very large sets and yet includes problem features that are realistic examples of actual applications. The specific case of linear, second order elliptic problems in two variables is considered and the components are given for a population with 425,000 members. This is based on 23 elliptic operators, 25 domains, 10 boundary operators and 74 true solutions. Most of the problem elements have 2 to 4 parameters so that a truly enormous population is constructed.

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1. OBJECTIVES

We present the design of a population of problems for the scientific evaluation of software for solving partial differential equations (PDEs). We consider the specific case of linear elliptic PDEs in two dimensions although the design may be extended to other classes (nonlinear, higher dimensions, etc.). An earlier population is given by [Rice, Houstis and Dyksen, 1981] and the use of it and other populations is discussed in [Rice, 1976], [Houstis, Lynch and Rice, 1978], [Boisvert, Houstis and Rice, 1979], [Rice, 1979], [Houstis and Rice, 1980] and [Dyksen, Houstis, Lynch and Rice, 1984].

One of the principal difficulties is to obtain a population of realistic problems which is large enough for statistical analysis. The population of [Rice, Houstis and Dyksen, 1981] is rather large (many problems have parameters) but once one starts specific studies one often sees that it is not large enough to obtain statistical results of high confidence levels. The design presented here dramatically increases the size of the population of problems by using a tensor product approach.

We provide the components for a tensor product population of second order, linear elliptic PDE problems in two variables with 425,000 members. Most of these have 1 to 4 parameters so as to create an enormous and varied population suitable for most experiments in the evaluation of PDE software in this problem domain.

2. THE DESIGN

We start by observing that a PDE problem is composed of four components:

1. The differential operator. We denote this operator by L and examples are

Laplace:	$u_{xx} + u_{yy}$
Helmholtz:	$u_{xx} + u_{yy} + au$
Other:	$(1 + x^2)u_{xx} + u_{yy} + x^2u_y + \sin(x + y)u$

We use the notation

$$Lu = a(x, y)u_{xx} + b(x, y)u_{xy} + c(x, y)u_{yy} + d(x, y)u_x + e(x, y)u_y + f(x, y)u$$

for linear operators in two variables. The differential equation is obtained by setting the operator equal to a given function $g(x, y)$, e.g. $Lu = g$ becomes

$$u_{xx} + u_{yy} = -1$$

2. The domain. We denote the domain by R and the differential equation is to be satisfied on R . That is, we want

$$Lu = g \quad \text{for all } x, y \in R.$$

Domains are normally open sets in the plane with simple boundaries defined by a few smooth curves. Examples are:

$$\text{The unit square: } 0 < x, y < 1$$

$$\text{The unit disk: } x^2 + y^2 < 1$$

3. Boundary operators. We denote these operators by B_i . They are defined on the boundary ∂R of the domain R and we consider ∂R to be made up of k pieces p_i , $i = 1, 2, \dots, k$ so that B_i is defined on p_i . Examples are

$$\text{Dirichlet: } u$$

$$\text{Neumann: } u_n \quad \text{the normal derivative}$$

$$\text{Other: } \cos(x)u_x + (1+x^2)u$$

The boundary conditions are obtained by setting the operator to given functions $h_i(x, y)$, e.g.

$$B_i u = h_i(x, y) \quad \text{for all } x, y \in p_i$$

4. Solutions: We denote these by $u(x, y)$. In constructing the population we choose the solution $u(x, y)$ and then compute the functions $g(x, y)$ and $h_i(x, y)$ which make $u(x, y)$ the true solution.

The PDE problem is thus to find $u(x, y)$ so that

$$\begin{aligned} L u &= g && \text{on } R \\ B_i u &= h_i && \text{on } p_i \in \partial R, i = 1, 2, \dots, k \end{aligned}$$

The idea of the tensor product approach to create a population of PDE problems is to create four populations, one each of differential operators = P_1 , domains = P_2 , boundary operators = P_3 and solutions = P_4 . The PDE population is then composed of sets $(L, R, \{B_i\}, u)$ where $L \in P_1, R \in P_2, \{B_i\}_{i=1}^k \in P_3$ and $u \in P_4$. Later we will describe population P_i with about 23, 25, 10 and 74 members, respectively, for $i = 1, 2, 3, 4$. This produces a population of PDE problems with about 400,000 members. Many members of these populations have one to four parameters which provides a truly enormous population.

There are two serious pitfalls which must be avoided in constructing these populations. The first is that arbitrary combinations may be illegal. Examples are:

(i) Let $L = u_{xx} + u_{yy}/(1+x/2)$

then $R = \text{unit square}$ produces a legal PDE

but $R = \text{unit disk}$ produces an illegal one.

(ii) Let $u(x, y) = \log(-.5 + x)$

then $R = \text{unit square}$ produces a legal PDE

but $R = \text{unit circle}$ produces an illegal one.

These examples and other similar ones suggest that: *The constituent populations P_1, P_3 and P_4 should involve functions which have no singularities.* This allows us to combine safely their elements with any domains.

Avoiding the first pitfall, singularities in the functions, exacerbates the second pitfall: *realistic problems have special behaviors associated with the domain geometry.* Obvious examples of this are corner singularities and boundary layers. Thus members of P_1 and P_4 (and perhaps P_3) must have some dependence on the domain in P_2 . Thus our design is to have these populations created from two subpopulations:

P_{1a}, P_{4a} = population dependent on R

P_{1b}, P_{4b} = population independent of R

We expect P_{1b} and P_{4a} to be much smaller than P_{1a} and P_{4b} . Then the elements of P_1 and P_4 are of the forms

$$P_1: L = L_a + L_b \quad L_a \in P_{1a}, \quad L_b \in P_{1b}$$

$$P_4: u = u_a + u_b \quad u_a \in P_{4a}, \quad u_b \in P_{4b}$$

The elements L_a and u_a depend explicitly on R , e.g.

$$L_a = \sqrt{r} u_{xx} + u_{yy} + s^{3/2} u$$

where

r = distance first corner point of boundary,

s = distance second piece of boundary.

Actual members of P_{1a} and P_{4a} are parametrized as illustrated by the following example for a solution in P_{4a} :

corner singularity:	corner number
	exponent of singularity
	size of singularity
boundary layer:	piece number
	decay exponent
	size of boundary layer
boundary singularity:	piece number
	exponent of singularity
	size of singularity

Simple specific examples of this construction are given in case the corner is $(0, 0)$, the boundary layer piece is $x = 0$ and the boundary singularity is $y = 0$:

Example 1:

$$u_a(x, y) = c_1(\sqrt{x^2 + y^2})^\alpha + c_2 e^{-\beta x} + c_3 y^\gamma$$

$$u(x, y) = u_a(x, y) + u_b(x, y)$$

where $u_b(x, y)$ is from P_{4b} and domain independent.

Example 2:

$$u_a(x, y) = c_4(x^2 + y^2)^{\alpha/2} e^{-\beta x} y^\gamma$$

$$u(x, y) = u_a(x, y) * u_b(x, y)$$

where $u_b(x, y)$ is from P_{4b} .

Finally, we note that in order to construct the functions $g(x, y)$ and $h_i(x, y)$ we need the partial derivatives of the solutions in P_4 . While this is straight forward in principle, it is a very tedious process to correctly compute all the required derivatives unless a symbolic algebra system is used. We assume the existence of a subroutine:

SUBROUTINE TDERIV (X, Y, TRUE, TRUEX, TRUEY, TRUEXX, TRUEXY, TRUEYY)

where TRUE, ..., TRUEYY are values of derivatives of the solution.

3. EXISTING COMPONENTS

In this section we summarize the status of the component populations P_1 , P_2 , P_3 and P_4 .

3.A. Differential Operators

The population of [Rice, Houstis and Dyksen, 1981] contains 56 linear elliptic operators.

These are numbered 1 to 56 and the following 29 are good candidates for P_1 :

1, 2, 4, 5, 6, 8, 9, 10, 11, 12, 17, 19, 20, 21, 22, 26, 30
31, 33, 34, 35, 38, 40, 41, 42, 43, 50, 53, 55

Of these, 11 are parametrized (12, 23, 26, 30, 39, 44, 45, 48, 49, 52 and 54). Some of these are similar; in particular, several are constant coefficient operators. Appendix P1 gives a set of 23 operators which are domain independent and which merges the constant coefficient cases into one. Additional parameters have been introduced into many additional differential operators.

3.B. Domains

The test set of [Rice, 1984a], [Rice, 1984b] provides 20 domains to test geometry processors in two dimensions. Three of these (9, 12 and 19) are quite complex and not very typical of domains appearing in PDE problems. This set has been extended by adding five more domains and by adding more parameters to some of the other domains. This new set is described in [Rice, 1986] which includes computer code definitions for all the domains. These domains are also incorporated into the ELLPACK system.

3.C. Boundary Operators

The population of [Rice, Houstis and Dyksen, 1981] contains many boundary condition operators, but only a few essentially different ones. This set is used as the basis for a new set of ten boundary operators given in Appendix P3.

3.D. Solutions

The population of [Rice, Houstis and Dyksen, 1981] contains many domain independent solutions (1, 2, 4, 5, 6, 8, 9, 10, 11, 12, 13, 17, 19, 20, 21, 22, 23, 24, 30, 31, 32, 33, 34, 35, 37, 38, 41, 42, 43, 50, 53, 54 and 56). These solutions are used as the basis of a new solution population with 37 members given in Appendix P4. Members 35, 36 and 37 give complex but fairly smooth behavior over a very large domain.

In [Rice, 1986] a domain dependent solution is given which provides singularities at specified boundary points and boundary layers along specified boundary pieces. Fortran code is included for it and its derivatives and this solution has been incorporated into the ELLPACK system. This one domain dependent solution can be combined with each of the 34 solutions in Appendix P4 to provide a total of 68 solutions.

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APPENDIX P1

A population of domain independent linear elliptic operators in two variables is given. These are derived from the population of PDE problems of [Rice, Houstis and Dyksen, 1981]. Parameters are denoted by $\alpha, \beta, \gamma, \dots$. These parameters may have to satisfy certain constraints so that the operators remain elliptic and non-singular. Certain known functions from [Rice, Houstis and Dyksen, 1981] are denoted by T and not specified exactly here.

1. $(e^{xy} u_x)_x + (e^{-xy} u_y)_y - 1/(1+x+y)u$
2. $u_{xx} + (1 + \alpha y^2)u_{yy} - \beta u_x + (1 + \alpha y^2)u_y$
3. $u_{xx} + u_{yy} - (\alpha + \cos(\pi\beta x) + \sin(\pi\gamma y))$
4. $u_{xx} + u_{yy} + (1 + \sin \alpha x)u_x - \cos \beta y u_y$
5. $(w u_x)_x + (w u_y)_y$ where $w = [T_x^2 + T_y^2]^\alpha, T = \text{known function}$
6. $u_{xx} + u_{yy} - e^T u$ where $T = \text{known function}$
7. $(1 + \alpha T^2)u_{xx} - \beta T^2 u_{xy} + (1 + \gamma T^2)u_{yy}$ where $T = \text{known function}$
8. $(w u_x)_x + (w u_y)_y$ where

$$w = \alpha \text{ if } A \leq 0.0025, \quad w = \beta + \gamma A \text{ if } A > 0.0025$$

$$A = \sqrt{T_x^2 + T_y^2}, \quad T = \text{known function}$$
9. $(w u_x)_x + (w u_y)_y$ where $w = 1/(\alpha + \beta A), A = \sqrt{T_x^2 + T_y^2},$
 $T = \text{known function}$
10. $(w u_x)_x + (w u_y)_y$ where $w = e^{A/(\alpha + \beta A)}/A, A = \sqrt{T_x^2 + T_y^2}$
 $T = \text{known function}$
11. $(w u_x)_x + (w u_y)_y$ where $w = \alpha \tanh(\beta A)/A, A = \sqrt{T_x^2 + T_y^2},$
 $T = \text{known function}$
12. $u_{xx} + u_{yy} + \beta(1+x^2)/(\alpha+x^2)^3 u_x$
13. $(2 + (y-1)e^{-\alpha y})u_{xx} + (1 + 1/(1 + |2x|^\beta))u_{yy} + \gamma(x(x-1) + (y-.3)(y-.7))u$
14. $(1 + \alpha T_y^2)u_{xx} - \beta T_x T_y u_{xy} + (1 + \alpha T_x^2)u_{yy}$ where $T = \text{known function}$
15. $u_{xx} + u_{yy} + \beta[1 - e^{\alpha x T^2}]u$ where $T = \text{known function}$
16. $u_{xx} + (1 + \alpha x^2)u_{yy} - \beta y u_y$
17. $u_{xx} + u_{yy} + w u$ where $w = -\alpha^2(1-T)^{\beta-1} e^{\gamma \beta T/(1+\gamma T)}, T = \text{known function}$
18. $u_{xx} + u_{yy} - \alpha T^{\beta-1} u$ where $T = \text{known function}$
19. $u_{xx} + u_{yy} - 1.425 T^{(\gamma-1)} e^{\alpha \beta (1-T) \gamma (1+\beta(1-T))} u$ where $T = \text{known function}$
20. $u_{xx} + u_{yy} + w$ where $w = -(1.425)^2 [(1 + \beta - T) \gamma \beta]^{\alpha-1} e^{\gamma T - 1/\gamma T}, T = \text{known function}$
21. $(w u_x)_x + (w u_y)_y - \alpha u$ where $w = 1/(1 + \beta T), T = \text{known function}$
22. $((1 + \beta x^2)u_x)_x + ((1 + A^2)u_y)_y - [1 + (\gamma y - x - 4)^2],$ where $A = 4y^2 + \alpha$
23. $\alpha u_{xx} + \beta u_{xy} + \gamma u_{yy} + \delta u_x + \eta u_y + \theta u$

APPENDIX P3

A population of domain independent boundary operators is given. Recall k is the number of pieces in ∂R and i is an index running from 1 to k . Parameters are denoted by $\alpha, \beta, \gamma, \dots$.

1. (Dirichlet) u
2. (Neumann) u_n
3. (Mixed) $\alpha u + \beta u_n$
4. $B_i u = u$ except for $i \neq j, B_j u = \alpha u + \beta u_n, j \leq k$
5. $B_i u = u$ except for $i \neq j1, j2, B_{j1} u = \alpha u + \beta u_n, j1, j2 \leq k$
 $B_{j2} u = \gamma u + \delta u_n$
6. $B_i u = \alpha_i u + \beta_i u_n$ for $i \neq j, B_j u = u, j \leq k$
7. $B_i u = u$ for $i \neq j, B_j u = \alpha u + \beta(y - y^2)u_n, j \leq k$
8. $B_i u = u$ for $i \neq j1, j2, B_{j1} u = \alpha u + \beta u_n$
 $B_{j2} u = \gamma u + \delta u_n$ where $\gamma\delta \equiv 0, \gamma + \delta = 1$ and γ, δ are unit step functions with step at η (in the parameter of piece $j2$)
9. $B_i u = u$ for $i = 1, i \geq 5, B_2 u = \alpha u + \beta u_n, B_3 = A u + B u_n$
 $B_4 u = C u + D u_n$ where p, q are the parameters of pieces 3 and 4 of ∂R and

$$A = \begin{cases} 1 & \text{for } p \leq \gamma \\ p & \text{for } p > \gamma \end{cases} \quad B = \begin{cases} 0 & \text{for } p \leq \gamma \\ 1 & \text{for } p > \gamma \end{cases}$$

$$C = \begin{cases} 0 & \text{for } q \leq \delta \\ q - \delta & \text{for } q > \delta \end{cases} \quad D = \begin{cases} 1 & \text{for } q \leq \delta \\ 1 + \delta - q & \text{for } q > \delta \end{cases}$$
10. $B_i u = u$ for $i \neq j1, j2, B_{j1} u = (1 + \cos(\alpha xy))u,$ $j1, j2 \leq k$
 $B_{j2} u = (1 + \beta \sin(x + y))u + u_n$

APPENDIX P4

A population of domain independent solutions is given. These are derived from the population of PDE problems given by [Rice, Houstis and Dyksen, 1981]. Parameters are denoted by $\alpha, \beta, \gamma, \dots$.

1. $e^{xy} \sin(\alpha\pi x) \cos(\beta\pi y)$
2. $(e^{x+y} + (x-\alpha)^2(x-\beta)^2) \log(1+y^2)$
3. $e^{x+y}(x-\alpha)(x-\beta)(y-\gamma)(y-\delta)$
4. $(x^2 - x)(\cos(\alpha\pi y) - 1)$
5. $(\alpha - C(x)) \sin(\beta\pi x)(y^2 - y)(\alpha - C(y)) [1/((1+\phi^4) - .5)]$ where $C(t) = \cos(\gamma\pi t)$, $\phi(x, y) = 4(x-.5)^2 + 4(y-.5)^2$
6. $\phi(x)\phi(y)$ where $\phi(t) = 1$ for $t \leq 0.5 - \alpha$, $\phi(t) = 0$ for $t \geq 0.5 + \alpha$, $\phi(t) = \text{quintic polynomial}$ for $0.5 - \alpha \leq t \leq 0.5 + \alpha$ so $\phi(t)$ has two continuous derivatives
7. $\cosh \beta x / \cosh \beta + \cosh \alpha y / \cosh \alpha$
8. $e^{-\alpha[(x-.5)^2 + (y-.5)^2]}(x-x^2)(y-y^2)$
9. $\sin[\alpha(x-y+2)^5/(1+(x-y+2)^4)]$
10. $\cos \alpha y + \sin \beta(x-y)$
11. $\min[x+\alpha, \beta+.5(x-.4) + (x-.4)^2/(1+x^2)](1+(y-1)^2e^{-y})$
12. $e^{(y^3 + (\alpha\beta x)^3/(1+(\beta x)^3)^3)} + \sin(x-y+.5)$
13. $\sin(\alpha\pi x) \sin(\beta\pi y)$
14. $\phi(x)\phi(y) + \alpha$ where $\phi(t) = e^{-\beta(t-.5)^2(t^2-t)}$
15. $e^{\alpha x + \beta y}$
16. $[\alpha + \beta(x^2 + y^2)](x^2 - 1)(y^2 - 1)$
17. $(\phi(y) + 1)\cos(\alpha\pi x)$ where $\phi(t) = 1$ for $t \leq 0.5 - \beta$, $\phi(t) = 0$ for $t \geq 0.5 + \beta$ and $\phi(t)$ is a quintic polynomial for $0.5 - \beta \leq t \leq 0.5 + \beta$ so $\phi(t)$ has two continuous derivatives.
18. $(x+y^2)/(1+|2x|^{\beta-1}) + (y-1)(1+x)e^{\alpha y} + \gamma(x+y)\cos(xy)$
19. $-(x^2+y^2)/4 + 0.821564 + 0.0144(x^4 - 6x^2y^2 + y^4) + 4.93 \times 10^{-5}(x^8 - 28x^6y^2 + 70x^4y^4 - 28x^2y^6 + y^8) - 6.4 \times 10^{-7}(x^{12} - 66x^{10}y^2 + 495x^8y^4 - 924x^6y^6 + 495x^4y^8 - 66x^2y^{10} + y^{12})$
20. $(1-y^2)(\alpha - 4x^2)(5-y^3)(y+\beta)$
21. $(1-y^2)[(1+\alpha)e^{\sqrt{\beta x}} + \gamma(1-y^2)e^{-\sqrt{\beta x}}]$
22. $.295776 - (x^2+y^2)/4 - 14476(x^4 - 6x^2y^2 + y^4)/319424 + 429(x^8 - 28x^6y^2 + 70x^4y^4 - 28x^2y^6 + y^8)/319424$
23. $\alpha + \beta[x^4 - 6x^2y^2 + y^4] + \gamma[x^8 - 28x^6y^2 + 70x^4y^4 - 28x^2y^6 + y^8]$
24. $(1-\beta)e^{x+y} + \beta \log(10^{-8} + |x+\alpha|)$
25. $(x-\alpha y)^2 e^{x-\beta y}$
26. $\cos[(2\alpha+1)x] \sinh[(2\alpha+1)y]$
27. $\log_{10}[10^{-8} + |(x+1)/\max(10^{-8}, 1+y)|] + \alpha e^{\beta(x+y)/(2+x-y)-2}$

28. $\frac{x(\pi-x)}{2} - \frac{4}{\pi} \sum_{j=1}^{\infty} \frac{\sin[(2j-1)x] \cosh[(2j-1)(y-\pi/2)]}{(2j-1)^3 \cosh[(2j-1)\pi/2]}$
29. $e^{-y/2} \sinh[5/4 + \gamma^2 \pi^2 / (\beta - \alpha)^2 y] \sin[\gamma \pi(x - \alpha) / (\beta - \alpha)]$, $\alpha \neq \beta$
30. $e^{\alpha(\pi-x)} \sinh \beta x \sin y$
31. $\alpha \sinh(1-y) \sin x + \beta \sinh 3(1-y) \sin 3x + \gamma \sinh \pi(1-x) \sin \pi y$
32. $\cos \beta y \sin(\alpha(x-y))$
33. $x(x-A(y))^2(1-e^{-\max\{0, (3-x/A(y))\}/\max\{0.02, x-A(y)\}})/A(y)^3 + \beta/(1+(8y-x-4)^2)$
where $A(y) = |4y^2 + \alpha| + 10^{-8}$
34. $\alpha + \beta x + \gamma x^2 + \delta x^3 + \eta x^4 + \varepsilon x^5 + \theta x^6$
35. $u(x, y) = T1(Z1(x, y, \alpha1, \beta1, \gamma1), Z2(x, y, \alpha2, \beta2, \gamma2) + .2, \delta1, \eta1)$
 $+ T2(Z2(x, y, \alpha3, \beta3, \gamma3), Z3(x, y, \alpha4, \beta4, \gamma4), \delta2, \eta2)$

where

$$\begin{aligned} T1(t, A, B, r) &= 1/(A + Bt^r) \\ T2(t, A, B, r) &= te^{-At}/(1 + B(t-r)^2) \\ Z1(x, y, A, B, r) &= \cos(x)^2 + \cos(y)^2/(1 + .6 \sin(Ax)) - r^2/(1 + .7 \sin(By)) \\ Z2(x, y, A, B, r) &= \sin(y) - \sin(Ax) + r \sin(2x \cos(By)) \\ Z3(x, y, A, B, r) &= \sin(y + A \sin(.7x)) \\ &\quad - r(1 + B \cos(.2x))/(\min\{1.5 - x^2/2, 1/\min(x, .1)\}) \end{aligned}$$

36. $u(x, y) = T1(\sqrt{x^2 + \sin(2xy)^2}, \delta1, Z3(x, y, \alpha1, \beta1, \gamma1), \eta1)$
 $+ T2(Z1(x, y, \alpha2, \beta2, \gamma2), \alpha3, \beta3, \gamma3)$
 $+ Z2(x, y, \alpha4, \beta4, \gamma4)$

where $T1, T2, Z2$ and $Z3$ are defined in solution 35.

37. $u(x, y) = Z1(x, y, \alpha1, \beta1, \gamma1)(1 + T1(Z3(x, y, \alpha2, \beta2, \gamma2), \alpha3, \beta3, \gamma3))$
 $+ \delta1 * Z2(x-y, x+y, \alpha4, \beta4, \gamma4) Z3(xy/\delta2, x-y, \alpha5, \beta5, \gamma5)$

where $T1, T2, Z2$ and $Z3$ are defined in problem 35.